

FIG. 1

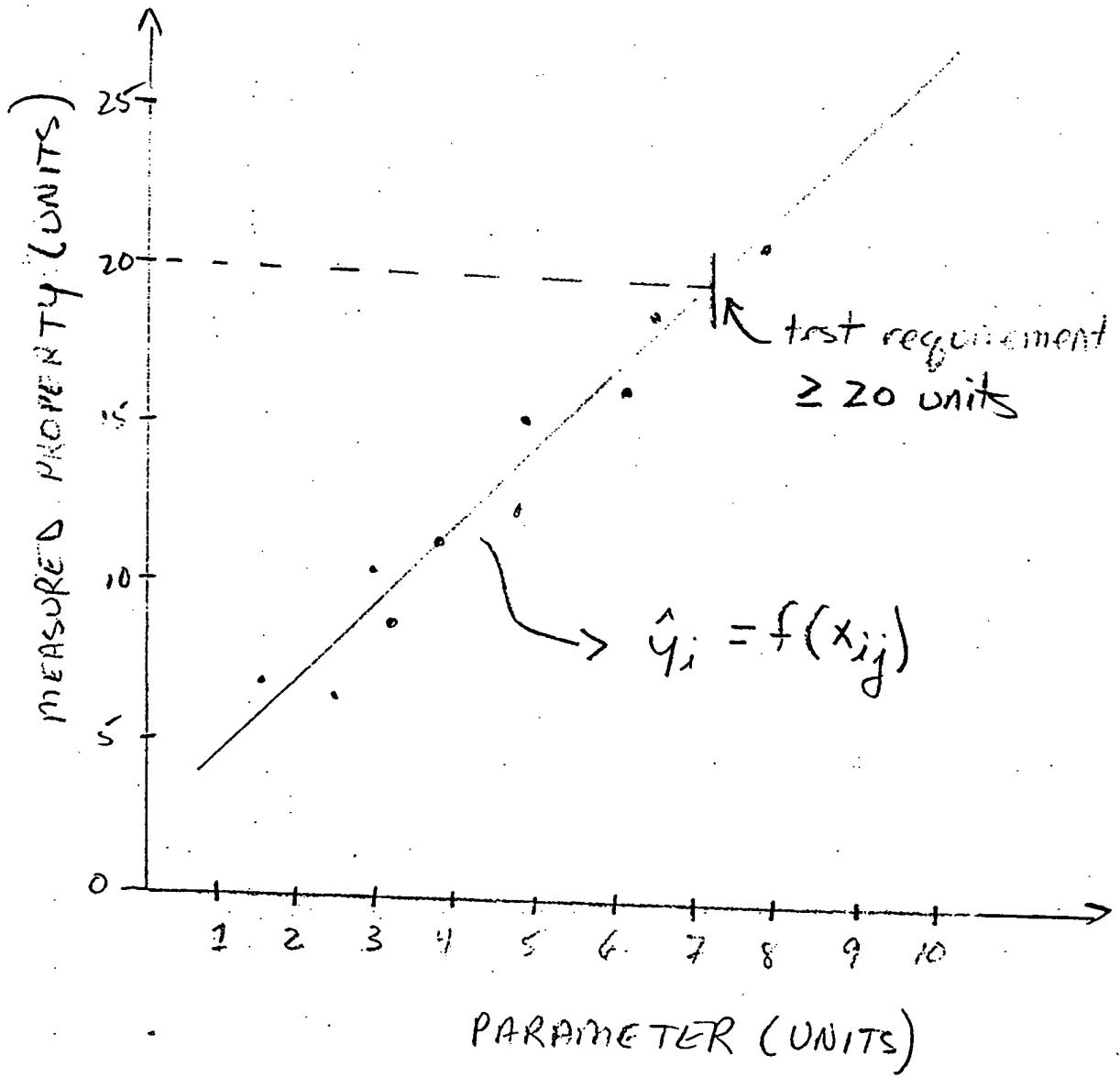


FIG. 2

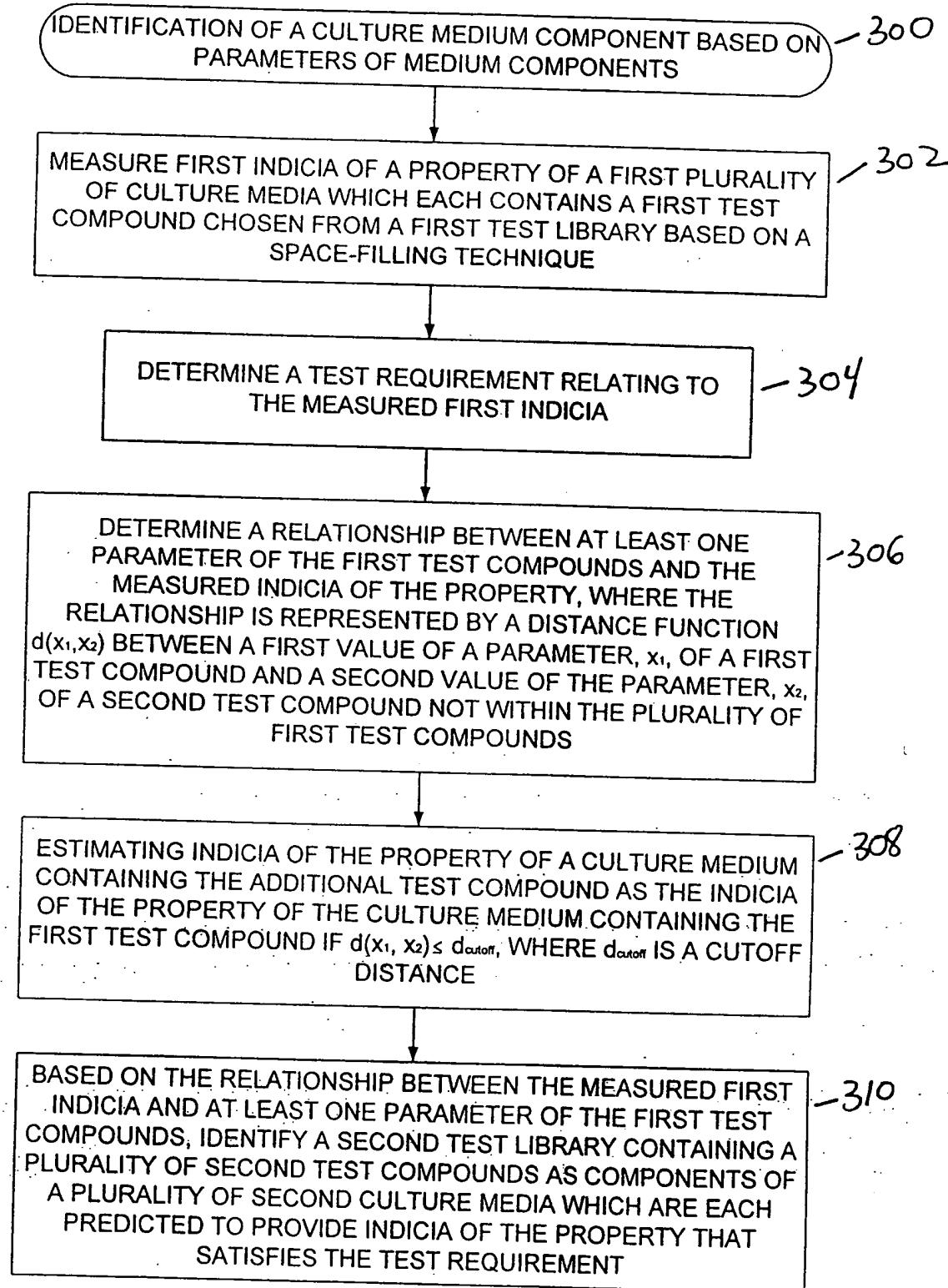


FIG. 3

IMPERFECT PROPERTY (UNITS)

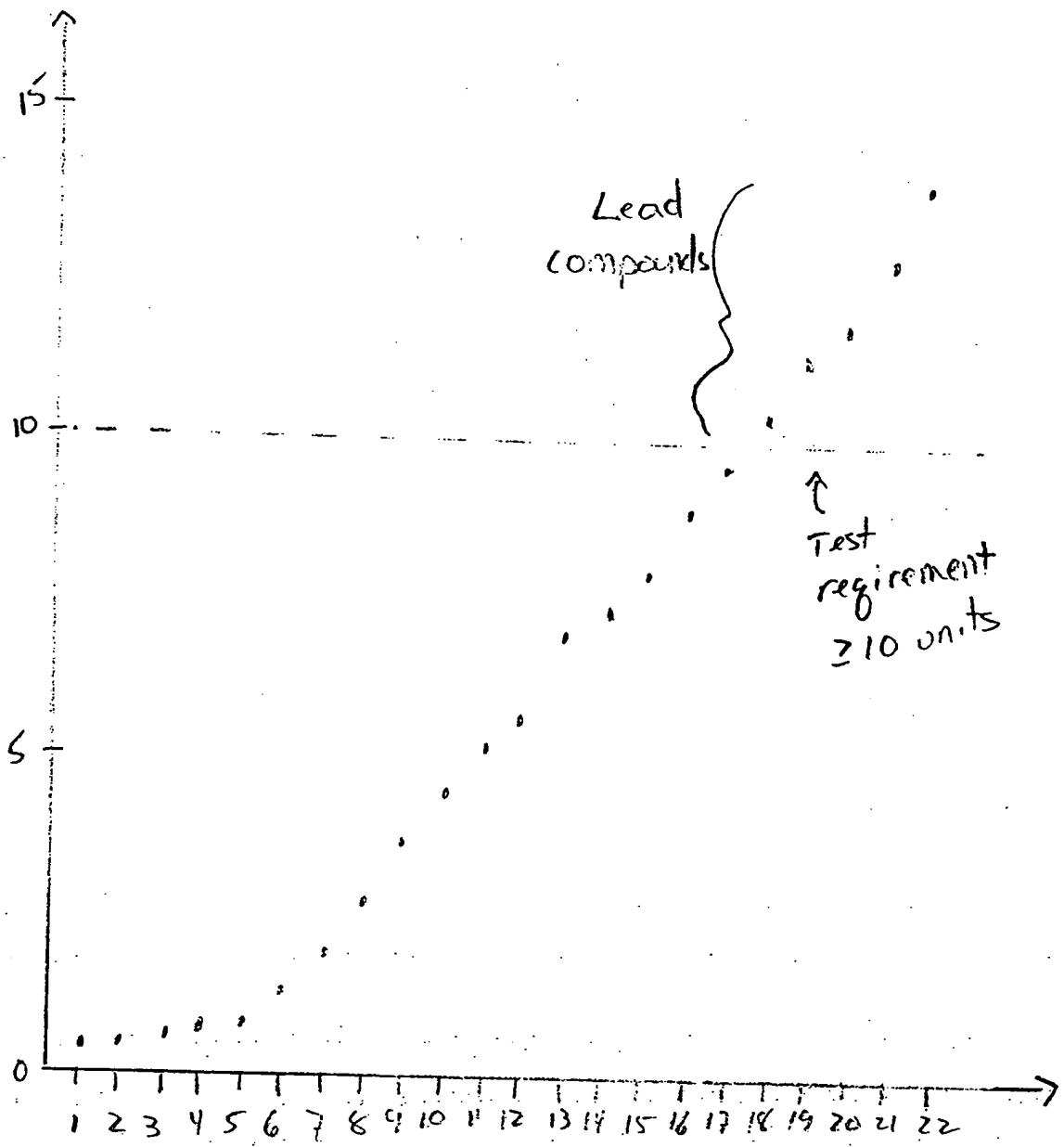


FIG. 4A

TOTAL DIPOLE

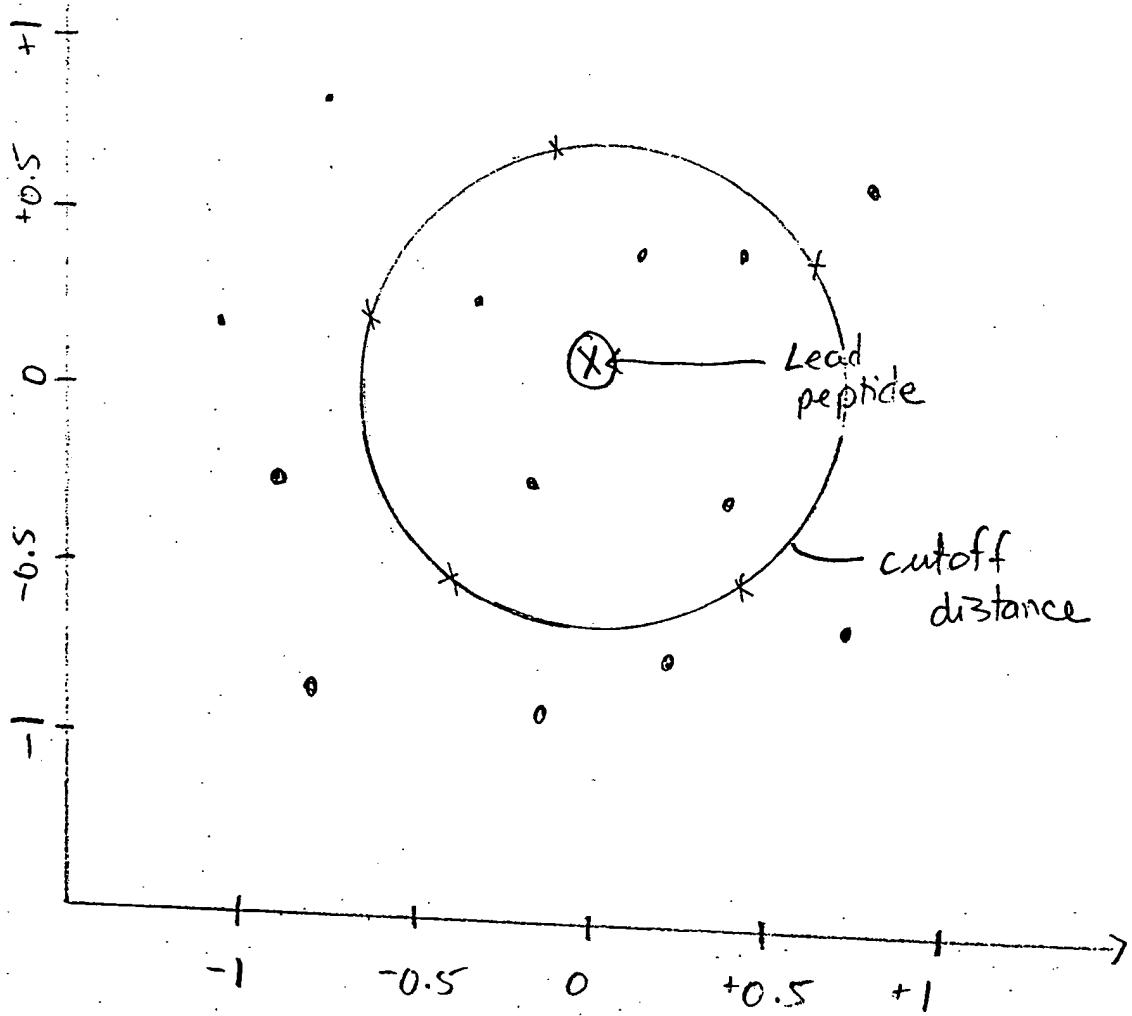


FIG. 4B

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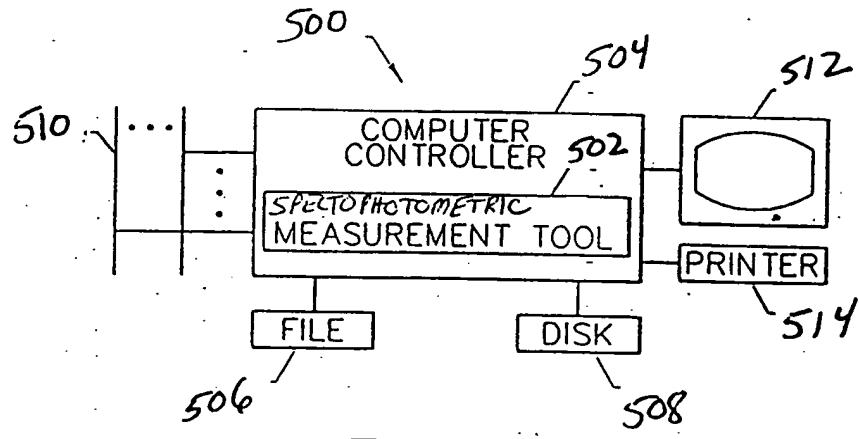


FIG. 5

60^c

FORMATION OF A REPRESENTATIVE COMPOUND LIBRARY BASED ON
WHOLE MOLECULE PARAMETERS

60²

REPRESENT EACH OF A PLURALITY OF GROUPS OF COMPOUND ISOMERS
FROM WITHIN A COMPOUND SPACE AS A RESPECTIVE CANDIDATE
COMPOUND BASED ON AT LEAST ONE SHARED GLOBAL PARAMETER

60⁴

EXPAND LESS THAN ALL OF THE CANDIDATE COMPOUNDS INTO THEIR
CONSTITUENT COMPOUND ISOMERS USING A SPACE-FILLING DESIGN

60⁶

DEFINE A TEST LIBRARY CONTAINING LESS THAN ALL OF THE EXPANDED
COMPOUND ISOMERS

FIG. 6

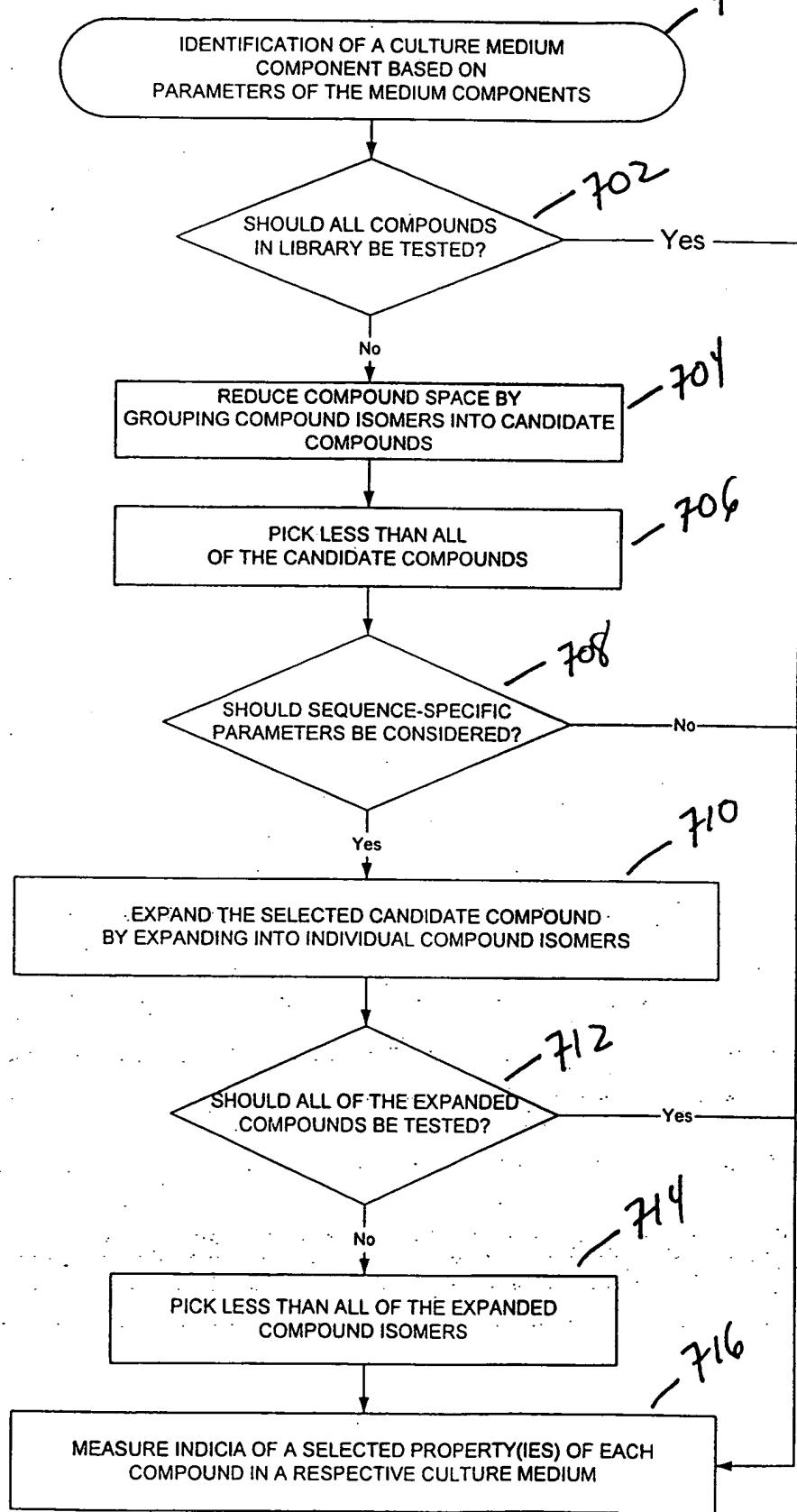


FIG. 7

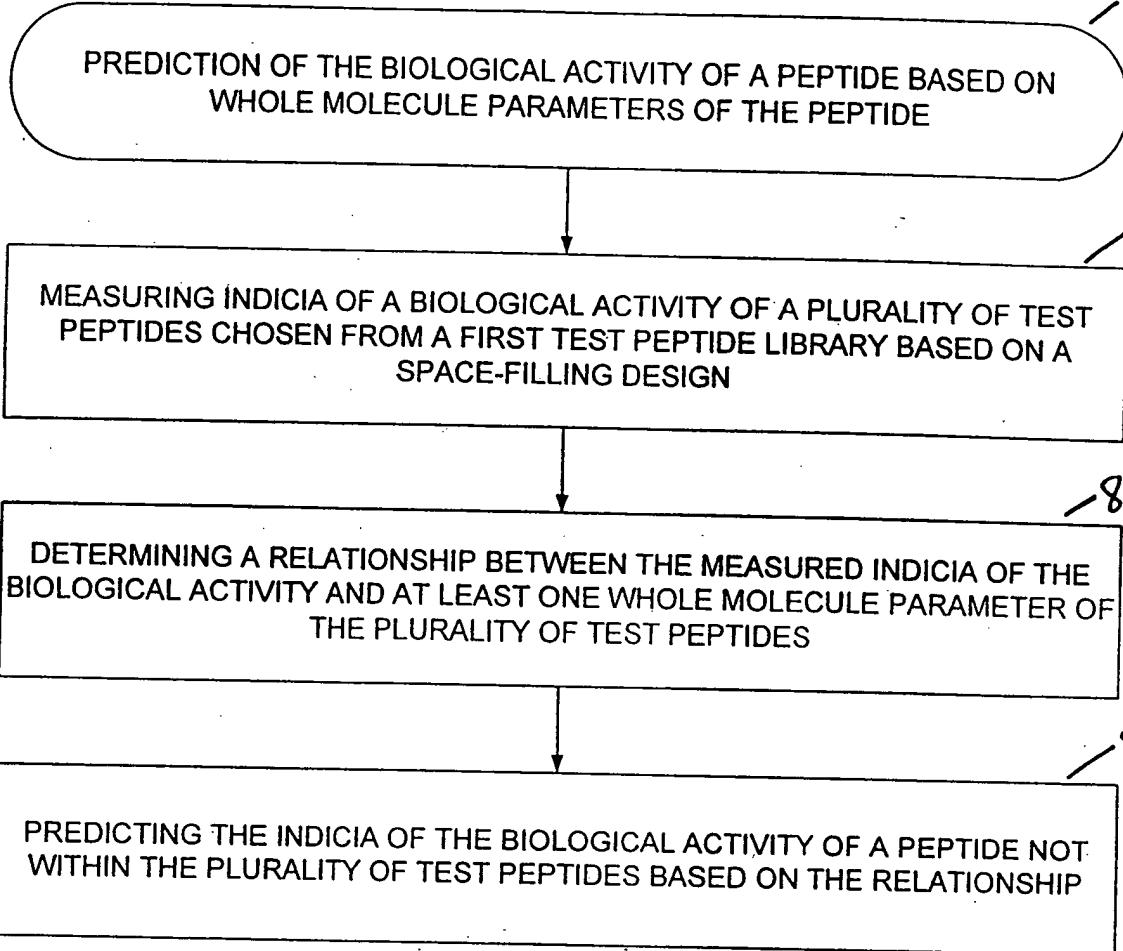


FIG. 8